ENGINEERING CHANGE NOTICE

1. ECN 635513

Proj. ECN

2. ECN Category (mark one) Supplemental [] Direct Revision [X] Change ECN [] Temporary [] Standby [] Supersedure [] Cancel/Void []	3. Originator's Name, Organization, MSIN, and Telephone No. John M. Conner, Data Assessment and Interpretation, R2-12, 373-2711	4. USQ Required? [] Yes [X] No	5. Date 07/25/97
	6. Project Title/No./Work Order No. Tank 241-S-111	7. Bldg./Sys./Fac. No. 241-S-111	8. Approval Designator N/A
	9. Document Numbers Changed by this ECN (includes sheet no. and rev.) HNF-SD-WM-ER-638, Rev. 0	10. Related ECN No(s). N/A	11. Related PO No. N/A

12a. Modification Work	12b. Work Package No.	12c. Modification Work Complete	12d. Restored to Original Condition (Temp. or Standby ECN only)
[] Yes (fill out Blk. 12b) [X] No (NA Blks. 12b, 12c, 12d)	N/A	N/A Design Authority/Cog. Engineer Signature & Date	N/A Design Authority/Cog. Engineer Signature & Date

13a. Description of Change

13b. Design Baseline Document? [] Yes [X] No

This ECN was generated to include additional explanatory text in the best-basis narrative, and to update the comprehensive radionuclide inventory estimates for the tank.

Rev. 0 pages included for duplicating purposes only.

14a. Justification (mark one)

Criteria Change	[]	Design Improvement	[X]	Environmental	[]	Facility Deactivation	[]
As-Found	[]	Facilitate Const	[]	Const. Error/Omission	[]	Design Error/Omission	[]

14b. Justification Details

Initial release of this document was deficient.

15. Distribution (include name, MSIN, and no. of copies)

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ENGINEERING CHANGE NOTICE

1. ECN (use no. from pg. 1) ECN-635513

16. Design Verification Required	17. Cost Impact				18. Schedule Impact (days)	
	ENGINEERING		CONSTRUCTION			
[] Yes	Additional	[] $	Additional	[] $	Improvement	[]
[X] No	Savings	[] $	Savings	[] $	Delay	[]

19. Change Impact Review: Indicate the related documents (other than the engineering documents identified on Side 1) that will be affected by the change described in Block 13. Enter the affected document number in Block 20.

SDD/DD	[]	Seismic/Stress Analysis	[]	Tank Calibration Manual	[]
Functional Design Criteria	[]	Stress/Design Report	[]	Health Physics Procedure	[]
Operating Specification	[]	Interface Control Drawing	[]	Spares Multiple Unit Listing	[]
Criticality Specification	[]	Calibration Procedure	[]	Test Procedures/Specification	[]
Conceptual Design Report	[]	Installation Procedure	[]	Component Index	[]
Equipment Spec.	[]	Maintenance Procedure	[]	ASME Coded Item	[]
Const. Spec.	[]	Engineering Procedure	[]	Human Factor Consideration	[]
Procurement Spec.	[]	Operating Instruction	[]	Computer Software	[]
Vendor Information	[]	Operating Procedure	[]	Electric Circuit Schedule	[]
OM Manual	[]	Operational Safety Requirement	[]	ICRS Procedure	[]
FSAR/SAR	[]	IEFD Drawing	[]	Process Control Manual/Plan	[]
Safety Equipment List	[]	Cell Arrangement Drawing	[]	Process Flow Chart	[]
Radiation Work Permit	[]	Essential Material Specification	[]	Purchase Requisition	[]
Environmental Impact Statement	[]	Fac. Proc. Samp. Schedule	[]	Tickler File	[]
Environmental Report	[]	Inspection Plan	[]		[]
Environmental Permit	[]	Inventory Adjustment Request	[]		[]

20. Other Affected Documents: (NOTE: Documents listed below will not be revised by this ECN.) Signatures below indicate that the signing organization has been notified of other affected documents listed below.

Document Number/Revision	Document Number/Revision	Document Number Revision
N/A		

21. Approvals

	Signature	Date		Signature	Date
Design Authority			Design Agent		
Cog. Eng. J.M. Conner	JM Conner	8-26-97	PE		
Cog. Mgr. K.M. Hall	Kathleen M Hall	8/26/97	QA		
QA			Safety		
Safety			Design		
Environ.			Environ.		
Other			Other		

DEPARTMENT OF ENERGY

Signature or a Control Number that tracks the Approval Signature

ADDITIONAL

Tank Characterization Report for Single-Shell Tank 241-S-111

John M. Conner
Lockheed Martin Hanford, Corp., Richland, WA 99352
U.S. Department of Energy Contract DE-AC06-96RL13200

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Key Words: Waste Characterization, Single-Shell Tank, SST, Tank 241-S-111, 241-S-111, S-111, S Farm, Tank Characterization Report, TCR, Waste Inventory, TPA Milestone M-44

Abstract: This document summarizes the information on the historical uses, present status, and the sampling and analysis results of waste stored in Tank 241-S-111. This report supports the requirements of the Tri-Party Agreement Milestone M-44-10.

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(2) Title
Tank Characterization Report for Single-Shell Tank 241-S-111

CHANGE CONTROL RECORD

(3) Revision	(4) Description of Change - Replace, Add, and Delete Pages	Authorized for Release (5) Cog. Engr.	(6) Cog. Mgr. Date
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		JMConner	Kathleen M. Hall 8/26/97

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3.0 BEST-BASIS STANDARD INVENTORY ESTIMATE

Information about the chemical and/or physical properties of tank wastes is used to perform safety analyses, engineering evaluations, and risk assessments associated with waste management activities, as well as to address regulatory issues. Waste management activities include overseeing tank farm operations and identifying, monitoring, and resolving safety issues associated with these operations and with the tank wastes. Disposal activities involve designing equipment, processes, and facilities for retrieving wastes and processing the wastes into a form suitable for long-term storage. Chemical inventory information generally is derived using two approaches: 1) component inventories are estimated using the results of sample analyses; and 2) component inventories are predicted using a model based on process knowledge and historical information. The most recent model was developed by Los Alamos National Laboratory (LANL) (Agnew et al. 1996). Not surprisingly, information derived from these two different approaches is often inconsistent.

An effort is underway to provide waste inventory estimates that will serve as standard characterization information for the various waste management activities (Kupfer et al. 1995). As part of this effort, an evaluation of available chemical information for tank 241-S-111 was performed that included an evaluation of available chemical information for tank 241-S-111 was performed, including the following:

- The inventory estimate generated by the Hanford defined waste (HDW) model (Agnew et al. 1996 and 1997)
- An engineering evaluation that produced a predicted concentrated supernatant solids (SMMS1) inventory based on a methodology developed by evaluating tanks 241-S-102, 241-S-102, 241-U-107, and 241-U-109.
- An engineering evaluation of REDOX sludge based on sampling-based data from tank 241-S-102, 241-S-104, and 241-S-107.
- Sample data from tank 241-S-111. Results of sample values are in Appendix B of this document.

Based on this evaluation, a best-basis inventory was developed for tank 241-S-111. For the following reasons, the sample-based evaluation inventory was chosen as the best basis for those analytes for which sampling-based analytical values were available.

- The sampling-based analytical concentrations of the other S and U tanks containing SMMS1 waste compared favorably with 241-S-111 sampling data.
- No methodology is available to fully predict SMMS1 saltcake from process flowsheet or historical records.

- No methodology is available to fully predict REDOX waste generated between 1952 and 1957 (R1) from process flowsheet or historical records for this tank. First-cycle R1 waste changed composition rapidly during the process, and accurate records of these changes are not available at this time. Also, R1 waste was cascaded and transferred into and out of many S, SX, and U tanks between 1972 and 1978, which makes it difficult to predict precipitation factors for analytes in the waste. Some tanks will show higher concentrations for certain analytes because of the length of time the waste was in the tank.

- In several cases, the sampling-based inventories do not support the assumptions and estimates made by the HDW model.

- For those few analytes for tank 241-S-111 where no data were available from the sampling or from the sampling-based inventory of similar tanks, the HDW model values were used with the notation that they were of lower reliability.

The best-basis inventory for tank 241-S-111 is presented in Tables 3-1 and 3-2. The deviation of the best-basis inventory is presented in Appendix D.

Table 3-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-S-111.

Analyte	Total Inventory (kg)	Basis (S, M, or E)[1]	Analyte	Total Inventory (kg)	Basis (S, M, or E)[1]
Al	254,000[2]	S	Ni	101	S
Bi	174	S	NO_2	91,900	S
Ca	497	S	NO_3	707,000	S
Cl	9,000	S	OH	n/r	
Cr	15,100	S	Pb	141	E
F	2,390	S	P as PO_4	25,300	S
Fe	575	S	Si	745	S
Hg	39.7	M	S as SO_4	52,000	S
K	2,330	S	Sr	232	E
La	98	E	TOC	6,600	S
Mn	151	S	U_{TOTAL}	639	S
Na	581,000	S	Zr	15	S

Notes:

n/r = not reported

[1]S = sample-based, M = HDW model-based, E = engineering assessment-based
[2] Based on fusion digest sample results

Table 3-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-S-111.[1]

Analyte	Total Inventory (Ci)	Basis (S, M, or E)[2]	Analyte	Total Inventory (Ci)	Basis (S, M, or E)[2]
^{3}H	556	M	^{226}Ra	5.80E-04	M
^{14}C	71.5	M	^{228}Ra	0.154	M
^{59}Ni	8.27	M	^{227}Ac	3.08E-03	M
^{60}Co	74.9	M	^{229}Th	3.66E-03	M
^{63}Ni	7.91	M	^{232}Th	0.0108	M
^{79}Se	729	M	^{231}Pa	8.81E-03	M
^{90}Sr	51,200	S	^{232}U	0.869	M
^{90}Y	51,200	S	^{233}U	3.33	M
^{93}Zr	35.7	M	^{234}U	2.32	M
^{93m}Nb	26.2	M	^{235}U	0.0964	M
^{99}Tc	511	M	^{236}U	0.0640	M
^{106}Ru	0.0125	M	^{238}U	2.42	M
^{113m}Cd	182	M	^{237}Np	1.96	M
^{125}Sb	313	M	^{238}Pu	5.34	M
^{126}Sn	11.0	M	^{239}Pu	281	M
^{129}I	0.984	M	^{240}Pu	42.12	M
^{134}Cs	3.91	M	^{241}Pu	332	M
^{137}Cs	4.18E+05	S	^{241}Am	2,530	E
^{137m}Ba	3.96E+05	S	^{242}Pu	1.65E-02	M
^{151}Sm	7.29	M	^{243}Am	3.75E-03	M
^{152}Eu	8.64	M	^{242}Cm	0.287	M
^{154}Eu	1220	M	^{243}Cm	0.0234	M
^{155}Eu	482	M	^{244}Cm	0.243	M

Notes:

n/r = not reported

[1]Radionuclides decayed to January 1, 1994

[2]S = sample-based, M = HDW model-based, E = engineering assessment-based

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APPENDIX D

EVALUATION TO ESTABLISH BEST-BASIS INVENTORY FOR SINGLE-SHELL TANK 241-S-111

An effort is underway to provide waste inventory estimates that will serve as standard characterization source terms for the various waste management activities (Hodgson and LeClair 1996). As part of this effort, an evaluation of available chemical information for tank 241-S-111 was performed, and a best-basis inventory was established. This work follows the methodology established by the standard inventory task.

D1.0 CHEMICAL INFORMATION SOURCES

- Sample data in Appendix B, core 149 segments 1 through 11.
- Samples from other S and U farm tanks with similar SMMS1 saltcake waste types.
- Sample data from other S farm tanks with R1 and CWR1 (REDOX cladding waste) sludge waste type.
- The HDW Model document (Agnew et al. 1996) provides tank content estimates in terms of component concentrations and inventories.

D2.0 COMPARISON OF COMPONENT INVENTORY VALUES

Tables D2-1 and D2-2 show HDW model inventories and sample data from tank 241-S-111. The waste volume used to generate the HDW inventory is 2,040 kL (538 kgal) total waste which is partitioned into 295 kL (78 kgal) sludge, 1,511 kL (399 kgal) saltcake, and 231 kL (61 kgal) unknown waste (Agnew et al. 1996). The HDW waste density was 1.59 g/mL.

The sampling-based inventory was generated using a solid waste volume of 1960 kL (517 kgal). The volume of liquid in the tank is less than 5 percent of the total volume, and the liquids will be pumped from the tank during stabilization activities. Therefore, only the solids were used to estimate the inventory. Waste volume estimates are described in Appendix A. The solids consist of 530 kL (139 kgal) of sludge and 1,430 kL (378 kgal) of saltcake. The derivation of the best-basis sampling inventory estimate is described in Section D4.2. The chemical species are reported without charge designation according to the best-basis inventory convention.

Table D2-1. Sample-Based and Hanford Defined Waste-Based Inventory Estimates for Nonradioactive Components in Tank 241-S-111.

Analyte	Sampling Inventory Estimate[1] (kg)	HDW[2] Inventory Estimate (kg)	Analyte	Sampling Inventory Estimate[1] (kg)	HDW[2] Inventory Estimate (kg)
Al	254,000	131,000	NO_3	707,000	597,000
Bi	174	316	OH	n/r	353,000
Ca	497	4,820	oxalate	17,300	1.85
Cd	17	n/r	Pb	n/r	1,410
Cl	9,000	13,700	P as PO_4	25,300	12,300
Cr	15,100	18,100	Si	745	4,210
F	2,390	1,600	S as SO_4	52,000	38,200
Fe	2390	15,300	Sr	14	0.718
Hg	n/r	39.7	TIC as CO_3	30,500	43,100
K	2,330	3,880	TOC	6,600	15,700
La	n/r	3.41	U_{total}	639	8,810
Mn	151	366	Zn	848	n/r
Mo	93	n/r	Zr	15	94
Na[3]	581,000	524,000	H_2O (Wt%)	28.7	36
Ni	101	1,440	Density (kg/L)	1.78	1.59
NO_2	91,900	263,000			

Notes:

[1]Sampling inventory calculated as described in Section D4.2.
[2]Agnew et al. (1996)

D3.5 BASIS FOR CALCULATIONS USED IN THIS ENGINEERING EVALUATION

Table D3-1 lists the approaches used for calculating and checking the supernatant, saltcake, and sludge inventories of tank 241-S-111.

Table D3-1. Engineering Evaluation Approaches Used On Tank 241-S-111.

Type of Waste	How Calculated	Check Method
Supernatant	Assumed no supernatant. (Although 87 kL [23 kgal] of supernatant is estimated, this liquid will be removed by salt well pumping.)	n/a
Saltcake Volume = 1,430 kL (378 kgal) Density = 1.68 g/mL	Used sampling based concentrations for tank 241-S-111.	SMMS1 average concentrations from other S and U Tank Farm tanks with sample data available.
Sludge Volume = 526 kL (139 kgal) Density = 1.67 g/mL	Used sampling based concentrations for tank 241-S-111.	Average sludge concentrations from other S Farm tanks with sample data available.

D3.5.1 Basis for Saltcake Calculations

The saltcake and sludge segment data for the tank 241-S-111 core sample were evaluated and compared to average concentrations of sample data from tanks with similar saltcake and sludge waste types. Based on extrusion observations and analytical data, the sample data for segments 4 through 8 were used to estimate the concentration of the saltcake layer. Data on the solids of segment 3 were excluded as less than 15 g were recovered. Data from Segment 9 were not used as this segment is transitional between the saltcake and sludge. The results for segments 4 through 8 were averaged to get the mean saltcake concentration for the tank, which was compared to analyses for other tanks using the check method described below.

The check method used is based on comparing data sets from S and U Tank Farm samples. Tanks 241-S-101, 241-S-102, 241-U-106, and 241-U-109 were used to produce the average saltcake analyte concentrations for SMMS1 saltcake. Agnew et al. (1996) indicates SMMS1 waste for all these tanks. To calculate the average SMMS1 concentration, the waste volumes and predicted location from the HDW model for the SMMS1 layer in each tank was determined. The TCR sample data was reviewed and using the segments located in the predicted location from the HDW model, an average concentration was calculated.

Table D3-2 shows the concentrations from each tank and the segments used in the calculation. The average component concentrations for the four tanks are also shown. For comparison, the SMMS1 saltcake composition predicted by the HDW model for tank 241-S-111 is shown.

Table D3-2. SMMS1 Saltcake Concentrations from Sampling Data and Modeling.[1] (2 sheets)

Analyte	S-101[2] Segments 2L-4U	S-102[2] Segments 7L-10U	U-106[2] Segments 2U-4L	U-109[2] Segments 5U-8L	Average of Tank Samples	S-111[2] Sample Segments 4-8	HDW Model SMM for S-111
Al	18,000	15,085	13,620	13,625	15,100	15,000	32,100
Ag	12	17	16	n/r	15	15	n/r
B	110	75	80	n/r	88	112	n/r
Bi	71	76	336	<DL[3]	161	60	113
Ca	273	237	336	<DL	282	148	881
Cl	4,500	4,099	2,926	3,560	3,770	2,980	4,790
Cr	10,000	4,359	3,170	4,233	5,440	5,470	2,430
F	500	13,600	4,669	298	4,840	972	575
Fe	508	1,298	3,096	<DL	1,630	222	270
K	1,109	898	1,309	n/r	1,110	811	1,360
La	<DL	37	43	n/r	40	n/r	n/r
Mn	266	597	1,189	<DL	684	54	131
Na	150,000	189,500	170,500	218,000	182,000	216,000	180,000
Ni	114	49	304	<DL	155	37	249
NO_2	91,000	40,100	56,000	42,900	57,502	30,500	85,600
NO_3	110,000	99,200	147,200	297,000	163,000	281,000	213,000
Pb	91	137	348	n/r	192	46	110
PO_4	9,500	114,500	5,888	5,970	34,000	9,140	4,400

analytical data on what was believed to be similar waste types. This tank also has analytical data from a 1996 sampling event. Thus, this engineering assessment provides an opportunity to compare data from the waste type formulation approach with the HDW model values and tank-specific analytical data.

Aluminum

Aluminum is expected to be in sludge and saltcake layers. The Al value for the four saltcake tanks shown in Table D3-2 is 15,100 μg/g. The sample based value is 15,000 μg/g agreeing with the values for the other tanks. The HDW SMM model value is 32,100 μg/g, a factor of two larger than either of the other two values. This factor has been seen in a number of S Tank Farm tanks. This may be caused by the lack of fusion data for the saltcake layers. Because of the lack of consistent fusion digest sample values, the analytical data is calculated on acid digest sample results. The sludge Al value is 249,000 μg/g (see Table D3-3) based on the fusion result. The analytical-based average concentration is 100,100 μg/g based on the average of acid digest sample results. The HDW model sludge concentration is 92,400 μg/g. The sample value is more then twice that of the other two values, which supports the conclusion that the sludge in tank 241-S-111 is mostly cladding waste.

Calcium

The HDW model predicts the Ca concentration would be approximately 6 times higher in the sludge than in the saltcake. However, both analytical and engineering assessment-based values indicate that the Ca concentrations are similar in saltcake and sludge. There appears to be considerably less Ca in the tank than predicted by the HDW model.

Chloride

The HDW model predicts the chloride concentration will be approximately 6 times higher in saltcake than in sludge. However, both the analytical data and the engineering assessment value predict that differences in chloride values between saltcake and sludge is less than a factor of two.

Chromium

In the sludge layer, there is agreement among the three concentration estimates for Cr. However, in the saltcake, the analytical value for Cr is approximately 2.7 times higher than the HDW model value. There is agreement between the engineering assessment value and the analytical value in the saltcake layer.

Iron

The analytical-based iron concentration in the sludge is far less than that predicted by the engineering assessment or the HDW model. The iron concentration predicted by the HDW model is approximately 690 times greater than the analytical-based value. The HDW model predicts R1 waste sludge in the tank, while the samples indicate that the sludge is cladding waste, which has considerably less iron.

Manganese

Potassium permanganate was used in the REDOX process until 1959; therefore manganese is expected to be in tanks containing waste from that process. Manganese is probably present as highly insoluble manganese dioxide in the alkaline waste materials and in the sludge. The R1/CWR1 sludge composition estimate developed in this engineering assessment for Mn was 1,330 μg/g. The SMMS1 saltcake composition estimate for Mn was 684 μg/g, much higher than would be expected based on solubility considerations. It should be noted that there are large ranges in the SMMS1 and R1 data sets for Mn. The HDW model predicts zero Mn in the sludge in tank 241-S-111 and 131 μg/g in the saltcake layer. Based on the analytical data, the Mn concentration in saltcake is 55 μg/g and in sludge 47 μg/g.

Phosphate

In the saltcake, a large difference exists between the engineering assessment concentration estimate and the HDW model and analytical-based estimates for phosphate. The engineering assessment value is biased high because of one extremely high phosphate value in data set used to develop the SMMS1 saltcake composition estimate (see Table D3-2). If the phosphate data from tank 241-S-102 are eliminated from the SMMS1 composition estimate, than the engineering assessment, analytical-based, and the HDW estimates would agree. The HDW model predicts zero phosphate in the sludge. The analytical-based and engineering assessment-based values are low (less than 2,000 μg/g phosphate).

Total Hydroxide.

Once the best-basis inventories were determined the hydroxide inventory was calculated by performing a charge balance with the valences of other analytes. In some cases this approach requires that other analyte (e.g., sodium or nitrate) inventories be adjusted to achieve the charge balance. During such adjustments, the number of significant figures is not increased. This charge balance approach is consistent with that used by Agnew et al. (1997).

D4.0 DEFINE THE BEST-BASIS AND ESTABLISH COMPONENT INVENTORIES

D4.1 OVERVIEW

As part of this effort, evaluations were performed of the following chemical information for tank 241-S-111:

- The inventory estimate generated by the HDW model (Agnew et al. 1996 and 1997).
- An engineering evaluation which produced a predicted SMMS1 inventory based on a methodology developed by evaluating tanks 241-S-102, 241-S-102, 241-U-107, and 241-U-109.
- An engineering evaluation of R1/CWR sludge based on sampling-based data from tanks 241-S-102, 241-S-104, and 241-S-107.
- Sample data from tank 241-S-111, reported in Appendix B.

Based on the evaluations, a best-basis inventory was developed for tank 241-S-111. Only one core was analyzed; therefore, the horizontal variability cannot be estimated. Variation between core samples (spatial variability) is often the largest source of variability in characterization samples (Jensen et al. 1995). Nevertheless and for the following reasons, the sample-based evaluation inventory was chosen as the best basis for those analytes for which sampling-based analytical values were available.

- The sampling-based inventory analytical concentrations of the other S and U tanks containing SMMS1 waste compared favorably with tank 241-S-111 sampling inventory.
- No methodology is available to fully predict SMMS1 saltcake from process flowsheet or historical records.
- Comparing sample-based sludge data from tank 241-S-111 to analytical data from other S Farm tanks provides strong evidence that the sludge in tank 241-S-111 is predominantly CWR rather than R1 waste.

D4.2 CALCULATION OF THE BEST-BASIS INVENTORY

The best-basis inventory is calculated using the mean saltcake and mean sludge concentrations for 241-S-111, presented in Tables D3-2 and D3-3. The volume of saltcake is assumed to be 1,430 kL (378 kgal) and the volume of sludge is assumed to be 526

(139 kgal), as estimated in Appendix A. The densities of saltcake and sludge are 1.68 and 1.67, respectively, derived from the sampling data for segments 4 through 8 for saltcake and 10 through 11 for sludge. The liquid data were not included in the inventory as the liquids will be pumped in the near future, and the volume of liquid is small relative to solids (less than 5 percent of total volume).

For certain analytes (total uranium and ^{90}Sr), data are only available from the core composite sample. The inventory for these analytes is calculated using the reported concentration, a solids volume of 1,957 kL (517 kgal), and a composite sample density of 1.78 g/mL. The inventory of ^{137}Cs is also calculated from the composite.

Certain other analytes were not measured analytically, or the results were below detection limits. For these, the engineering assessment or HDW model estimates were used. Tables D4-1 and D4-2 show the best-basis inventory for tank 241-S-111. The source of the data is listed for each analyte. The inventory values reported in Tables D4-1 and D4-2 are subject to change. Refer to the Tank Characterization Database for the most current inventory values.

Best-basis tank inventory values are derived for 46 key radionuclides (as defined in Section 3.1 of Kupfer et al. 1997), all decayed to a common report date of January 1, 1994. Often, waste sample analyses have only reported ^{90}SR, ^{137}Cs, $^{239/240}Pu$, and total uranium, or (total beta and total alpha) while other key radionuclides such as ^{60}Co, ^{99}Tc, ^{129}I, ^{154}Eu, ^{155}Eu, and ^{241}Am etc., were infrequently reported. For this reason, it was necessary to derive most of the 46 key radionuclides by computer models. These models estimate radionuclide activity in batches of reactor fuel, account for the split of radionuclides to various separations plant waste streams, and track their movement with tank waste transactions. (These computer models are described in Kupfer et al. 1997, Section 6.1 and in Watrous and Wootan 1997). Model generated values for radionuclides in any of the 177 tanks are reported in Agnew et al. (1997). The best-basis value for any one analyte may be a model result, a sample, or an engineering assessment-based result, if available. (No attempt has been made to ratio or normalize model results for all 46 radionuclides when values for measured radionuclides disagree with the model). For a discussion of typical error between model-derived values and sample-derived values, see Kupfer et al. (1997, Section 6.1.10).

Table D4-1. Best-Basis Inventory Estimates for Nonradioactive Components in Tank 241-S-111.

Analyte	Total Inventory (kg)	Basis (S, M, or E)[1]	Analyte	Total Inventory (kg)	Basis (S, M, or E)[1]
Al	254,000[2]	S	Ni	101	S
Bi	174	S	NO_2	91,900	S
Ca	497	S	NO_3	707,000	S
Cl	9,000	S	OH	n/r	
Cr	15,100	S	Pb	141	E
F	2,390	S	P as PO_4	25,300	S
Fe	575	S	Si	745	S
Hg	39.7	M	S as SO_4	52,000	S
K	2,330	S	Sr	232	E
La	98	E	TOC	6,600	S
Mn	151	S	U_{TOTAL}	639	S
Na	581,000	S	Zr	15	S

Notes:

[1]S = sample-based, M = HDW model-based, E = engineering assessment-based

[2]Based on fusion digest sample results

Table D4-2. Best-Basis Inventory Estimates for Radioactive Components in Tank 241-S-111.[1]

Analyte	Total Inventory (Ci)	Basis (S, M, or E)[2]	Analyte	Total Inventory (Ci)	Basis (S, M, or E)[2]
^{3}H	556	M	^{226}Ra	5.80E-04	M
^{14}C	71.5	M	^{228}Ra	0.154	M
^{59}Ni	8.27	M	^{227}Ac	3.08E-03	M
^{60}Co	74.9	M	^{231}Pa	8.81E-03	M
^{63}Ni	791	M	^{229}Th	3.66E-03	M
^{79}Se	7.29	M	^{232}Th	0.0108	M
^{90}Sr	51,200	S	^{232}U	0.869	M
^{90}Y	51,200	S	^{233}U	3.33	M
^{93}Zr	35.7	M	^{234}U	2.32	M
^{93m}Nb	26.2	M	^{235}U	0.0964	M
^{99}Tc	511	M	^{236}U	0.0640	M
^{106}Ru	0.0125	M	^{238}U	2.42	M
^{113m}Cd	182	M	^{237}Np	1.96	M
^{125}Sb	313	M	^{238}Pu	5.34	M
^{126}Sn	11.0	M	^{239}Pu	281	M
^{129}I	0.984	M	^{240}Pu	42.2	M
^{134}Cs	3.91	M	^{241}Pu	332	M
^{137}Cs	4.18E+05	S	^{242}Pu	1.65E-03	M
^{137m}Ba	3.96E+05	S	^{241}Am	2,530	E
^{151}Sm	7.29	M	^{243}Am	3.75E-03	M
^{152}Eu	8.64	M	^{242}Cm	0.287	M
^{154}Eu	1220	M	^{243}Cm	0.0234	M
^{155}Eu	482	M	^{244}Cm	0.243	M

Notes:

[1]Radionuclides decayed to January 1, 1994

[2]S = sample-based, M = HDW model-based, E = engineering assessment-based

D5.0 APPENDIX D REFERENCES

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